U.S. Department of Energy

Advancing Mission Through Science

Presentation to the National Geospatial Intelligence Agency

NGA Chief Scientist Colloquium Series

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Elements of Successful Programs

Successful programs in the DOE Office of Science have the following features:

- Address mission needs
- Seize scientific opportunities that push the frontiers of current understanding and the tools necessary to do so
- Involve community participation in road-mapping
- Openly competed among universities, national labs, and the private sector
- Attract the best Principal Investigators in the field
- Externally peer reviewed – both prospectively and retrospectively to ensure quality
- Visionary and bold program managers willing to take risks
- Uncompromising philosophy of world leadership

Examples of recent successes:

- **Leadership Computing**
- **DOE Bioenergy Research Centers**
- **Pushed the frontiers of science at the nanoscale, systems biology, catalysis, materials**
- **Established large scientific user facilities for the Nation – SNS, RHIC, NSRCs**
- **Developed major detectors for U.S. scientific programs at the LHC – the future energy frontier for high energy physics**

SNS: Spallation Neutron Source (Oak Ridge); RHIC: Relativistic Heavy Ion Collider (Brookhaven); NSRCs: Nanoscale Science Research Centers (5 centers); LHC: Large Hadron Collider (CERN)

Mission-driven Science

Like the Department of Energy, the National Geospatial Intelligence Agency is a mission agency with technical challenges that can be met through support of mission-driven science and technology research.

Establishing Long-Term Research Directions at DOE's Office of Science

- **DOE Mission Needs**

  Energy security, national security, science-driven technology

- **Workshops**

  Engaging the broader scientific community to identify opportunities

- **Scientific Advisory Committees**

  Independent advice and external review of programs and management

- **National Priorities**

  Nanotechnology, high-speed computing, advanced energy, climate change, U.S. competitiveness and innovation

Our Energy Challenge

Essential Role of Basic Research for DOE's mission

- **Today's energy technologies and infrastructure are rooted in 20th Century technologies and 19th Century discoveries—internal combustion engine, incandescent lighting, alternating current transmission lines.**
- Current fossil energy sources, current energy production methods, and current technologies cannot meet the energy challenges we now face.
- Incremental changes in technology will not suffice. We need **transformational discoveries** and **disruptive technologies.**

Science Transforming Energy Technologies

Imagine:

- Solar photovoltaics exceeding thermodynamic efficiency limits
- Direct conversion of sunlight to chemical fuels
- Solar and wind providing over 30% of electricity consumed in the U.S.—enabled by better electrical energy storage.
- A closed nuclear fuel cycle and abundant fossil-free power with zero greenhouse gas emissions
- Bringing the power of the sun and the stars to Earth with fusion energy
- A sustainable, carbon-neutral biofuels economy that meets over 30% of U.S. transportation fuel needs without competing with food, feed, or export demands.

DOE Leadership Computing

Vision and Commitment

In science of the 21st century, simulation and high-end computing are equal partners with theory and experiment.

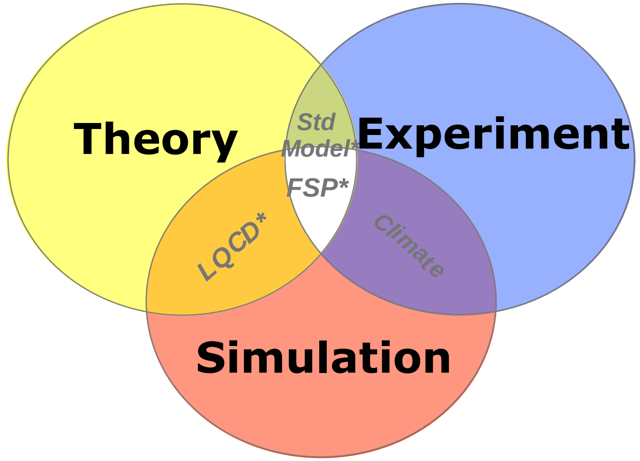
Six years ago:

- The largest computer available to the DOE Office of Science was the NERSC facility at 3 teraflops peak
- Our highest sustained speed on, for example, fusion codes was 485 Gigaflops (<16% peak)
- Our ESnet could transfer data at 622 megabits per second
- We just started the Scientific Discovery through Advanced Scientific Computing (SciDAC) program in 2001

In the Spring of 2002 we were awestruck by the great accomplishment of the Japanese with their Earth Simulator. This opened our eyes to the possibility of doing things on a scale and more rapidly than we had ever imagined before.

Our Vision:

The *Three Pillars of Scientific Discovery*



**Std Model =Standard Model of Particles and Interactions*
**FSP =Fusion Simulation Project*
**LQCD =Lattice Quantum Chromodynamics*

In 2003, we announced the DOE vision for scientific computing with the Leadership Computing Facilities (LCF).

- The LCFs would be open to all, including industry, and prioritize access based peer review – similar to the light sources and particle colliders the DOE had provided for decades
- Two LCFs were established: Oak Ridge National Laboratory and Argonne National Laboratory
- NERSC (National Energy Research Scientific Computing Center at Lawrence Berkeley Laboratory) upgraded
- Access to computing facilities made available through the INCITE program

INCITE: Innovation and Novel Computational Impact on Theory and Experiment

DOE Leadership Computing

Vision and Commitment

We've come a long way in 6 years:

- 104 teraflop Cray XT4 at NERSC
- 263 teraflop Cray XT4 at Oak Ridge (One petaflop acquired by the end of 2008)
- 100 teraflop IBM Blue Gene/P (500 teraflop IBM Blue Gene/P running by the end of 2008)
- ESnet will be at 40 gigabits per second core in 2008 and 60 Ggbs in the Metropolitan Area Networks
- Efficiencies on some problems (codes) are as much 75%
- The SciDAC program supports universities and laboratory researchers and centers that bring scientists together with applied mathematicians and computer scientists to develop the scientific applications that will run affectively on the HPC platforms
- The INCITE program will award 265 million CPU hours in 2008 and over half a billion CPU hours in 2009
- Computation and simulation projects have delivered remarkable results for science

What enabled this success:

- Although computing can change a lot in five years, we did not waiver from our vision and commitment to realizing high performance computing as a third pillar for scientific discovery
- Excellent program managers and senior management that continued to support the vision, even in budget-challenged years
- Excellent project management at HQ and the facility sites
- Continued input from the community through scientific meetings and peer review panels guided decisions for pursuit of the best science

DOE Leadership Computing

Vision and Commitment

Looking ahead: Exascale

- In less than 10 years, computers utilizing massive multi-core chips will achieve peak speeds 1,000 times a petaflop (an exaflop).
- Effective use of exascale systems will require fundamental changes in how we develop and validate simulation codes for these systems and how we manage and extract knowledge from the massive amounts of data produced.
- In 2007, we hosted three town hall meetings around the country to pulse the community about areas of science that need more computing capabilities to achieve their goals.
- We are making long-term investments, one in partnership with DARPA, to push the frontiers of computing architectures.
- At the same time, we are investing in the applied mathematics and computer science needed to bring scientific applications to petascale and beyond, recognizing that exascale architectures necessitate radical changes to the software used to operate them and the science applications—the change is as disruptive as the shift from vector to distributed memory supercomputers 15 years ago.

DOE Bioenergy Research Centers

Timely Response to Scientific Opportunity and National Priorities

- The capability to tap into the energy contained in plant fiber or cellulose would give us the means to produce biofuels on a scale sufficient to create a nationwide biofuels economy that would not compete with food or feed crops. But current methods for converting cellulose to sugars and other metabolites that can be used to produce fuels are not economically viable.
- Emerging tools of systems biology can be used to help overcome current obstacles to bioprocessing cellulosic feedstocks to ethanol and other biofuels – metagenomics, synthetic biology, high-throughput screening, advanced imaging, and high-end computational modeling.

Several factors contributed to DOE's ability to successfully launch three new Bioenergy Research Centers in 2007 to tackle the scientific and technical challenges to cellulosic biofuels:

- Through several workshops over four years, the scientific community built the case for the role of systems biology and biotechnology for developing solutions to DOE's energy and environmental challenges. In 2006, DOE released a detailed scientific roadmap, produced by the systems biology community and facilitated by Office of Science program managers, for a compelling research program focused on biofuels: *Breaking the Biological Barriers to Cellulosic Ethanol.*
- Two presidential initiatives were announced in January 2006: the Advanced Energy Initiative (AEI) and the American Competitiveness Initiative (ACI) that called for increased funding for this area of research.
- A National Academy of Sciences report endorsing the Office of Science systems biology program recommended the department establish "vertically integrated" research centers focused on DOE mission areas, beginning with bioenergy.
- In August 2006, DOE called for bioenergy research center proposals in a Funding Opportunity Announcement that was open to universities, national laboratories, the private sector, or partnerships among those groups.

DOE Bioenergy Research Centers

Timely Response to Scientific Opportunity and National Priorities

- The open FOA enabled the Nation's best scientific talent to come together to propose ideas for a center focused on cracking Nature's code for cost-effective biofuel conversion – the response was impressive.
- Three centers were selected for award based on a rigorous merit review process by an external review panel of experts. Each center is awarded $25M per year for five years.

  DOE BioEnergy Science Center – led by Oak Ridge National Laboratory, includes 9 partnering institutions.

  DOE Great Lakes Bioenergy Research Center – led by University of Wisconsin-Madison in partnership with Michigan State University, includes 6 other partnering institutions.

  DOE Joint BioEnergy Institute – led by Lawrence Berkeley National Laboratory, includes 5 other partnering institutions.

- The Office of Science held a review of the centers' management plans (with external reviewers) three months after first funds were released to ensure centers got started on the right foot.
- All three centers were up and running by the end of 2007.
- Each center, as part of its research proposal and management plan, identified research and technology milestones; the centers will be reviewed annually on the progress towards these milestones.
- The lead institutions' tech transfer arrangements and partnerships with industry enable the centers to effectively move basic research discoveries to applications.

Basic and Applied Research for Mission Need

The future technologies to meet mission needs require innovation and revolutionary leaps in current understanding that can only come from basic research – grand challenge, discovery, and "use-inspired" research.

Strong coordination and communication is required across the basic and applied programs.

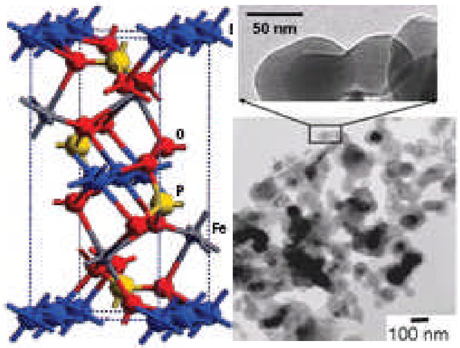
- Coordination efforts informed by community input, driven at the program manager level, integrated into the annual budget and planning process, and supported by senior management have a greater likelihood of success.
- Applied research programs must strive to maintain adequate support of longer-term applied research even under pressure to support more technology demonstration and deployment.

Li-ion Batteries

Basic to Applied Example in Electrical Energy Storage

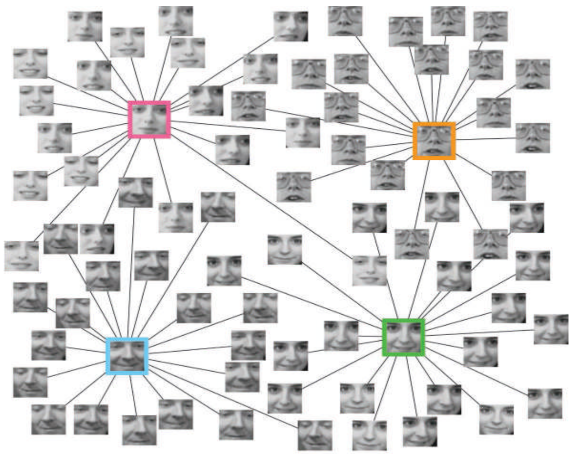
Electrical energy storage (EES) devices with substantially higher energy and power densities and faster recharge times are needed if such technologies as all-electric/plug-in hybrid vehicles are to be deployed broadly.

- The Office of Science Office of Basic Energy Sciences supported fundamental studies of the electronic conductivity of $LiFePO_4$ which led to the discovery of doping-induced conductivity increases of eight orders of magnitude and the concept for nanostructured electrodes with tailored architectures.
- This research discovery enabled the research group (which formed A123 Systems) to successfully compete in DOE's Small Business Innovation Research (SBIR) program supported by the DOE Office of Energy Efficiency and Renewable Energy (EERE), one of DOE's applied technology programs.
- The research supported by the SBIR program and EERE led to the development of high power-density Li-ion batteries by A123 Systems to power electric vehicles such as the Chevy Volt and the Th!nk.



$LiFePO_4$ structural model and nanostructure

Seizing Opportunities



Faces in a crowd. Exemplars (highlighted by colored boxes) have been detected from a group of faces by affinity propagation.

Caravaggio's "Vocazione di San Matteo." How to choose an exemplar through message passing. The messages are exchanged in the directions of the fingers and of the glances, leading to the recognition of San Matteo as the "exemplar."

M. Mézard, Science, 315, p.949; Frey and Dueck, Science, 315, p.972-6 (2007)

The next generation of tools and instruments for mission needs will come from new discoveries – must be ready to seize them

Example: A new computational method for finding an optimal set of data clusters to manage large, noisy data sets using exemplars.

- The algorithm detects special data points (exemplars) and connects every data point to the exemplar that best represents it
- Uses affinity propagation – a message-passing algorithm – a powerful method for extracting representative data from complex data sets such as images
- Has potential for broad applications in pattern recognition

Risk-Taking and Long-term Commitment

- Reaching beyond current paradigms and technologies to accomplish mission needs necessarily requires risk-taking and supporting "high-risk, high-return" research.
- The DOE Office of Science programs view high-risk, high-return research as an integral part of their research portfolios and essential for achieving the scientific breakthroughs needed to meet program goals.
- Peer review provides a rigorous evaluation of the quality of the science and the merit of a proposal; it is program managers – subject-matter experts in their fields – who weigh the results of peer review with risk and potential impact on program missions to determine funding recommendations.
- Discoveries from basic and "use-inspired" research, and applications of that research, rarely occur on in the short-term so a commitment to long-term investment is necessary as well as mechanisms for continuous identification of new scientific opportunities.
- Regular reviews of research projects and research portfolios help identify problems and enables early course-correction.

Engaging the Scientific Community in the Mission

Engaging the Nation's scientific and technical talent in an agency's mission arguably provides the greatest impact to mission goals

Roles of the scientific community

- Identify scientific opportunities and help prioritize compelling research directions
- Provide expert review of research proposals for quality, merit, and relevance
- Provide external review of research portfolios for scientific excellence (Federal Advisory Committees)
- Provide external review of program management practices (Committee of Visitors)
- Provide needed diversity of perspectives
- Bring to bear their scientific talent, leadership, and dedication to mission-relevant research and development and train the next generation of scientists who are inspired to do the same

Agencies cannot obtain diversity of thought or maximize the impact the scientific community can have on mission goals without operating in an open science environment